

# MEMS Gas-Chromatograph Pre-Concentrator Multiphysics Simulation

MEMS Gas-Chromatograph (GC) is a key system for a miniaturized planetary (Mars) atmospheric life detector [1]. A methodology is shown to optimize the preconcentrator MEMS chip design. The chip absorbs VOCs in Tenax<sup>®</sup> layer and fast desorbs them by heating. This development was funded by ESA.

G. Spinola Durante, A. Hoogerwerf, D. Bayat Zaman

Swiss Center for Electronics and Microtechnology (CSEM), Neuchâtel,

#### Introduction

The objective of this simulation model is to enhance the thermal behavior of a MEMS Gas-Chromatograph (GC) pre-concentrator of Volatile Organic Compounds (VOCs).

Precise and rapid temperature control is essential for optimal VOC desorption from the Tenax<sup>®</sup> polymer filling the pre-concentrator chip cavity. By inducing a fast-heating pulse, we release highly time-concentrated VOCs into the carrier gas (Helium) exiting the pre-concentrator, leading to increased accuracy of VOCs detection.

The simulation plays a critical role in estimating the heater geometry, its maximum voltage and current density, thermal time constants, and spatial temperature uniformity within the Tenax<sup>®</sup> polymer material. The chip design optimization comes with a few challenges i.e. voltage is limited to 28V and current must be lower than the heater electro-migration limit. Tenax<sup>®</sup> temperature uniformity is reduced by heatsinking of the chip to its surroundings. Chip size is limited due to yield & costs issues. Tenax<sup>®</sup> target heating is 280-300°C in <5s in >70% volume.



## Methodology

Thermal and flow models required experimental validation of material properties of Tenax<sup>®</sup> porous material pellets. A flow model has been implemented with calibrated parameters based on the heating setup of a cube filled with Tenax<sup>®</sup>. Gas-flow behavior of Tenax<sup>®</sup> porous material has been estimated based on literature flow data for a round pipe filled with Tenax<sup>®</sup> particles and accordingly simulated and calibrated with a model [2, 3]. Selected physics have been included in the chip model: heat transfer in solid and fluids, laminar flow, with porous flow in Tenax<sup>®</sup> and electrical current in shells (2D-layer) to model the pre-concentrator heater. The selected physics are also coupled together to correctly compute ohmic losses in the heater and non-isothermal flow due to strong thermal gradients in the model as shown in Fig. 1 (a, b).

FIGURE 1 (a, b). MEMS pre-concentrator chip temperature, (c): optimized heater current density.

### Results

The model solves in 1h40m on a Linux<sup>®</sup> Server and helps to quantify the Tenax<sup>®</sup> spatial (volume) and temporal temperature evolution in form of relative volume histogram snapshots for specific time-slices. The initial symmetric heater and thermal connection design was delivering 30% of Tenax<sup>®</sup> temperature uniformity in 20°C range, around the peak. It gave insight how to effectively optimize the asymmetric heater design, its position on chip and resulted in Tenax<sup>®</sup> heating speed-up reaching a range of 265-285°C in ~2.5s within >64% of the volume (Fig. 2a). The heater is operated at a power of ~27W. A different Tenax<sup>®</sup> configuration, based on same chip size and heater improved the Tenax<sup>®</sup> heating range of 275-295°C in ~3.1s within >84% of the volume (Fig. 2b). Finally, the heater is operating with a current density of ~3E5A/cm2 and well below the limit (Fig. 1c).



FIGURE 2 (a). Tenax<sup>®</sup> temperature distribution optimized, (b): Tenax<sup>®</sup> temperature distribution improved uniformity.



Excerpt from the Proceedings of the COMSOL Conference 2024 Florence

#### REFERENCES

1. High-performance MEMS-based gas chromatography column with integrated micro heater https://link.springer.com/article/10.1007/s00542-010-1165-y

2. Tenax<sup>®</sup> TA Adsorbent Resin Specifications

https://www.sisweb.com/index/referenc/tenaxtam.htm#4

3. COMSOL Blog: Modeling Darcian and Non-Darcian Flow in Porous Media https://www.comsol.com/blogs/modeling-darcian-and-non-darcian-flow-in-porous-media